

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
 Data File : VN072109.D
 Acq On : 21 Apr 2022 04:43
 Operator : JC\MD
 Sample : N2482-14
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SPN-9

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
 Title : SW846 8260

Signal : TIC: VN072109.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	37	47	62	rVB5	39306	154133	4.21%	0.636%
2	2.440	72	77	87	rVB	40261	71348	1.95%	0.294%
3	3.134	185	195	207	rVB	378468	869187	23.72%	3.586%
4	3.998	332	342	351	rBV	30470	77696	2.12%	0.321%
5	4.287	375	391	409	rBV2	30788	116321	3.17%	0.480%
6	4.581	432	441	454	rBV2	11514	37423	1.02%	0.154%
7	5.081	513	526	533	rBV4	46790	182310	4.98%	0.752%
8	5.187	533	544	568	rVB4	92462	415746	11.35%	1.715%
9	5.622	604	618	631	rBV3	33953	118063	3.22%	0.487%
10	6.469	753	762	771	rVB2	12931	37370	1.02%	0.154%
11	6.610	775	786	795	rBV3	13232	38652	1.05%	0.159%
12	6.904	825	836	845	rBV2	19702	54165	1.48%	0.223%
13	7.145	861	877	884	rBV3	129449	394803	10.77%	1.629%
14	7.216	884	889	902	rVB3	65538	170222	4.65%	0.702%
15	7.410	915	922	932	rVB2	18708	49228	1.34%	0.203%
16	7.845	987	996	1007	rVB	52442	131819	3.60%	0.544%
17	8.022	1015	1026	1031	rBV	442875	1098692	29.98%	4.533%
18	8.080	1031	1036	1048	rVB	869525	1991319	54.35%	8.216%
19	8.445	1087	1098	1112	rBV3	684731	2064127	56.33%	8.516%
20	8.586	1112	1122	1124	rBV7	18356	49717	1.36%	0.205%
21	8.963	1177	1186	1200	rBV	1270167	2649201	72.30%	10.930%
22	9.245	1229	1234	1240	rVB	20971	41052	1.12%	0.169%
23	9.969	1350	1357	1362	rBV2	44167	86121	2.35%	0.355%
24	10.322	1409	1417	1422	rBV	22372	39464	1.08%	0.163%
25	10.439	1428	1437	1445	rBV	1994312	3664181	100.00%	15.117%
26	10.639	1464	1471	1477	rBV2	98373	173426	4.73%	0.716%
27	10.710	1477	1483	1493	rVB	98643	178593	4.87%	0.737%
28	11.739	1650	1658	1670	rBV	1925836	3407167	92.99%	14.057%
29	11.839	1670	1675	1685	rVB	41978	77841	2.12%	0.321%
30	11.951	1688	1694	1701	rVB	44638	86739	2.37%	0.358%
31	12.574	1792	1800	1809	rVB	118046	196654	5.37%	0.811%
32	12.727	1818	1826	1841	rBV	1401908	2387535	65.16%	9.850%
33	12.915	1852	1858	1864	rBV	100279	164868	4.50%	0.680%
34	13.668	1978	1986	1999	rBV	1511833	2575665	70.29%	10.626%
35	13.874	2015	2021	2036	rVB	191645	340631	9.30%	1.405%
36	14.321	2092	2097	2103	rVB3	28289	46769	1.28%	0.193%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Title : SW846 8260

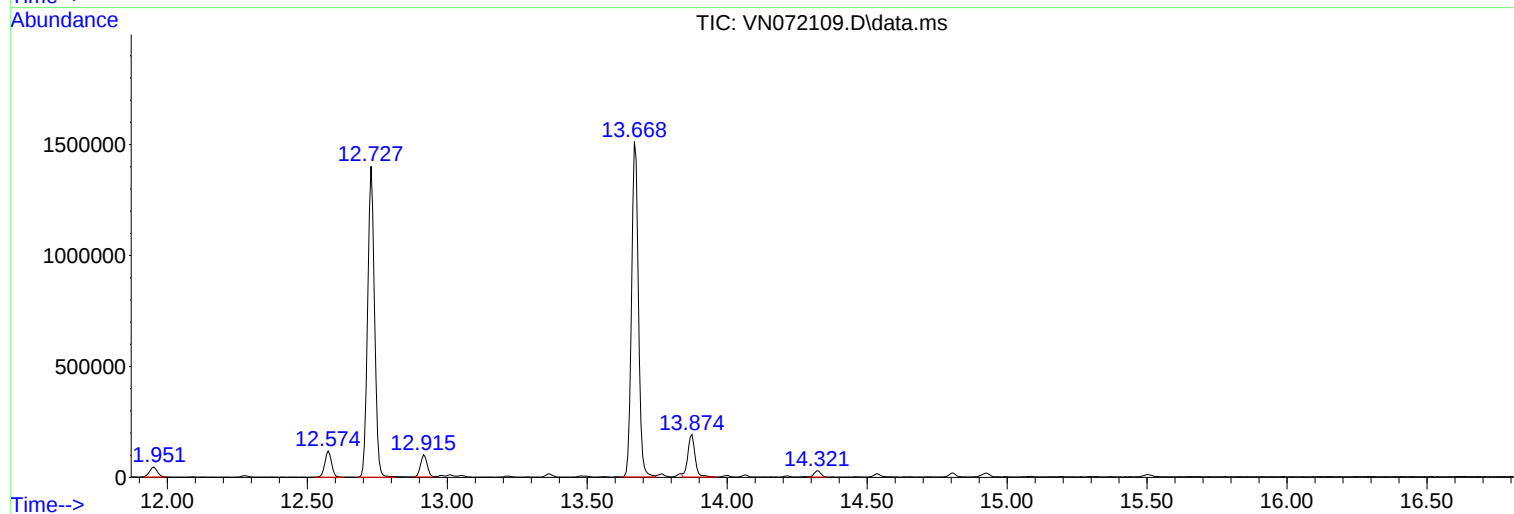
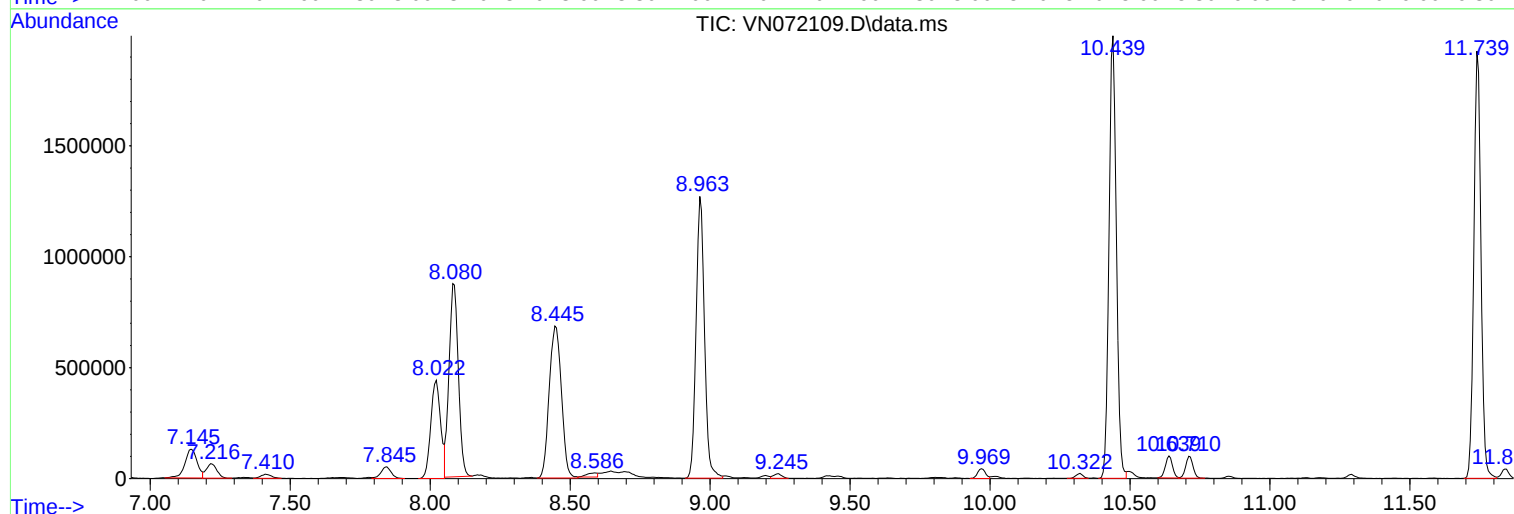
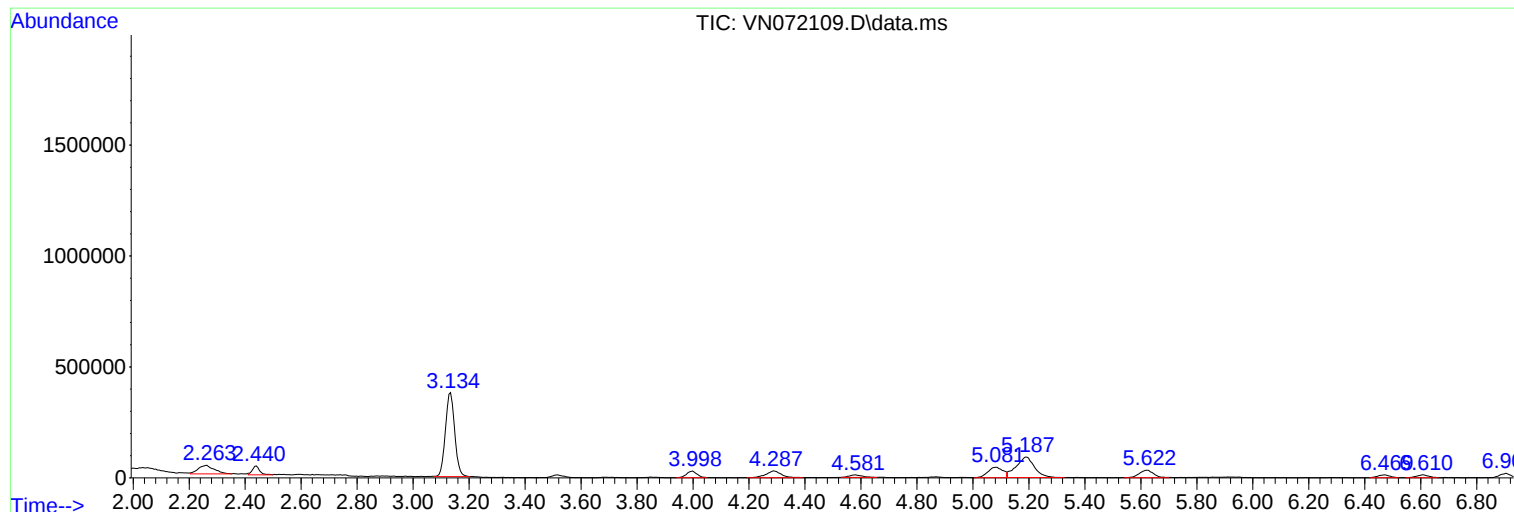
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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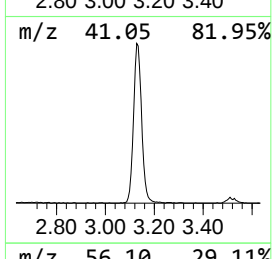
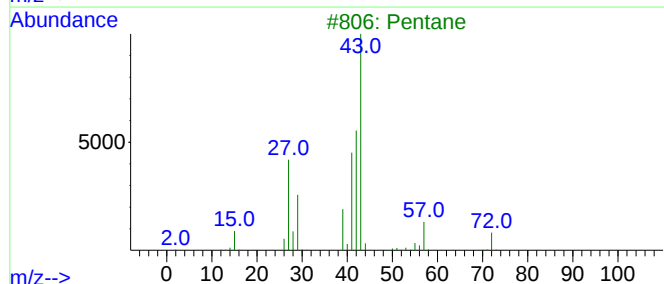
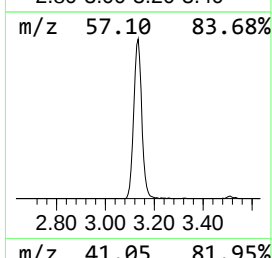
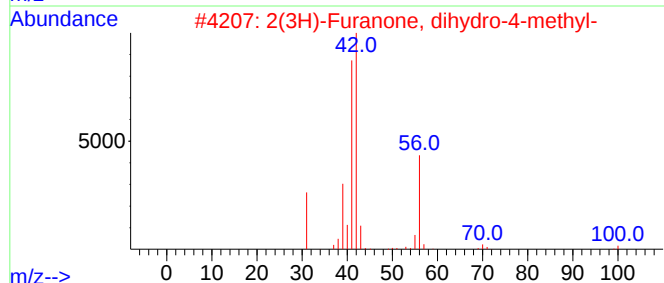
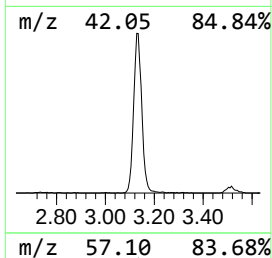
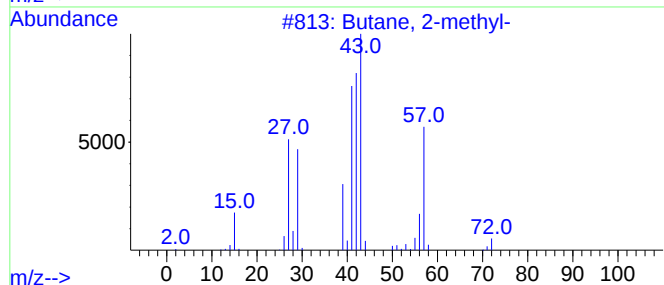
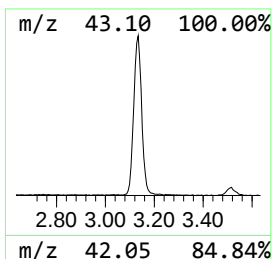
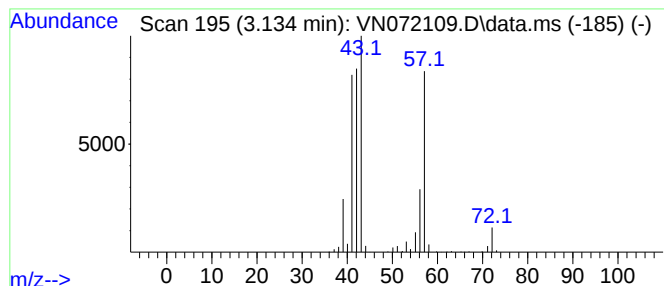
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	21.82 ug/l	869187	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	36
3			Pentane	72	C5H12	000109-66-0	33
4			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	12
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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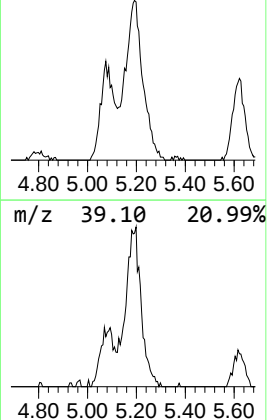
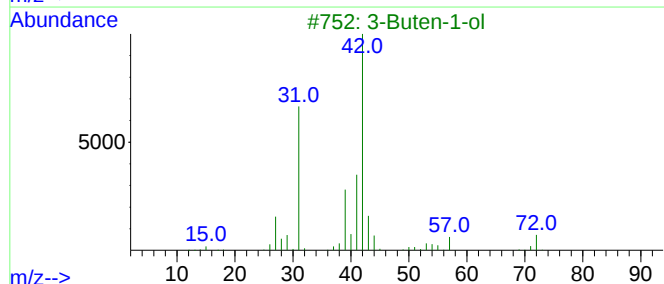
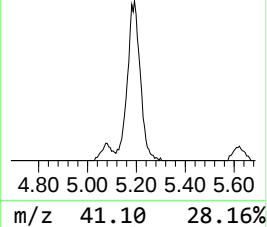
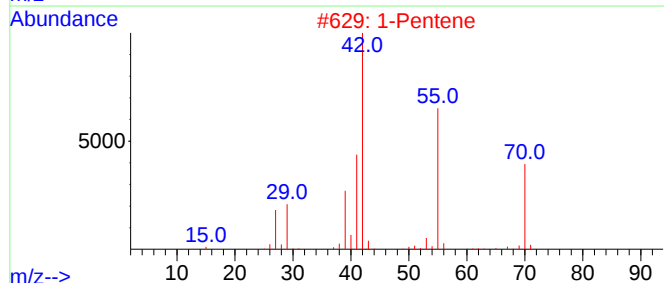
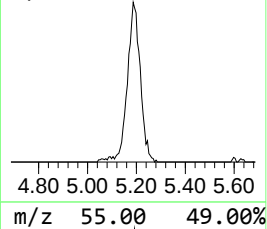
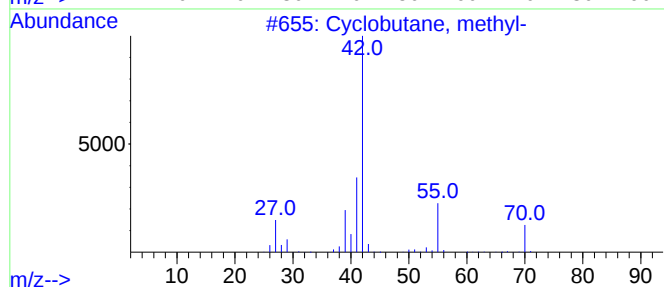
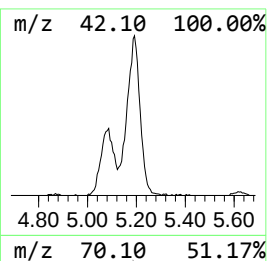
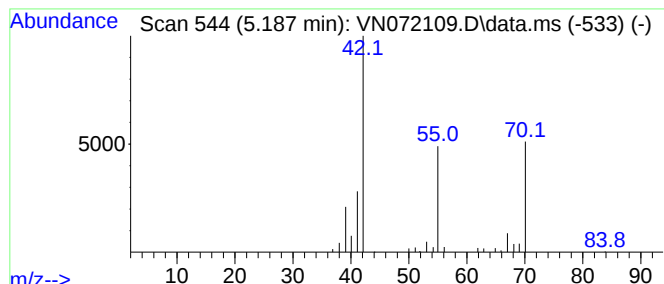
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclobutane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	10.44 ug/l	415746	Pentafluorobenzene	8.080

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclobutane, methyl-	70	C5H10	000598-61-8	72
2		1-Pentene	70	C5H10	000109-67-1	39
3		3-Buten-1-ol	72	C4H8O	000627-27-0	28
4		Isobutyronitrile	69	C4H7N	000078-82-0	9
5		Cyclopentane	70	C5H10	000287-92-3	9



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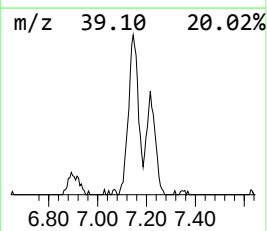
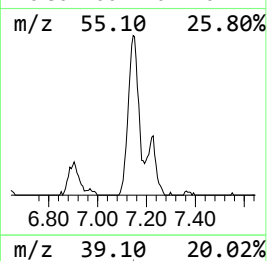
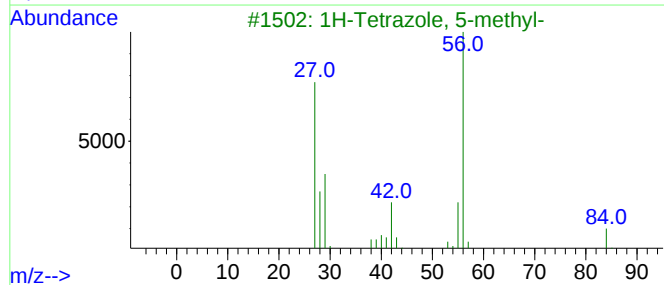
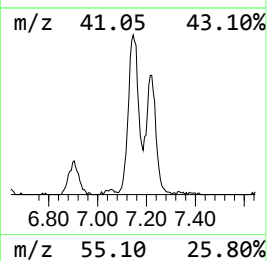
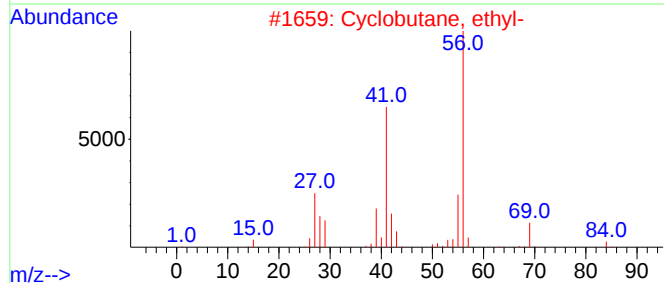
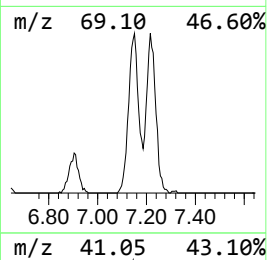
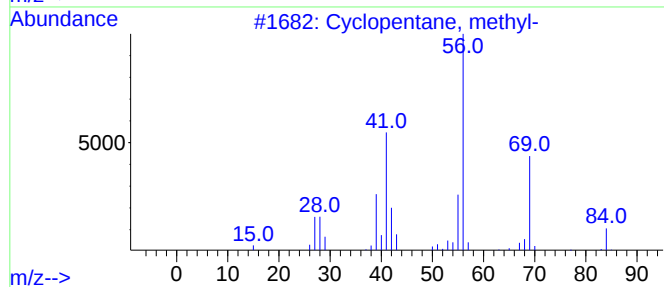
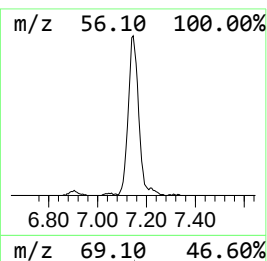
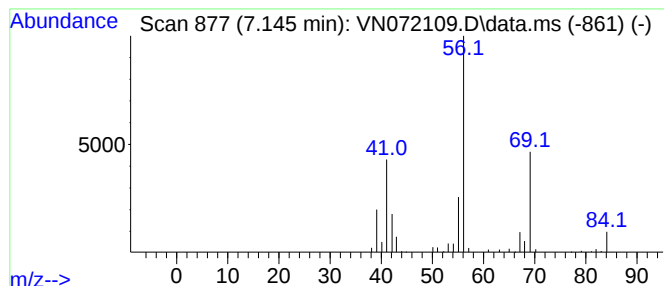
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	9.91 ug/l	394803	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
4			Cyclohexane	84	C6H12	000110-82-7	47
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	46



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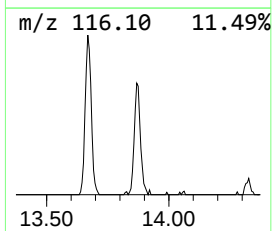
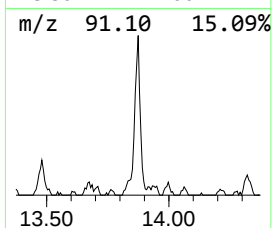
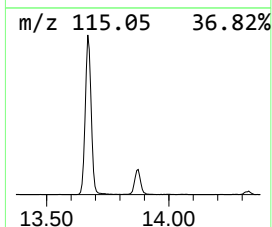
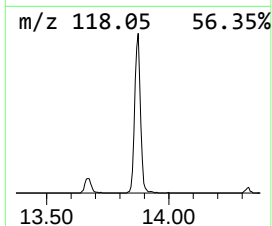
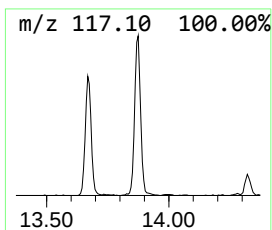
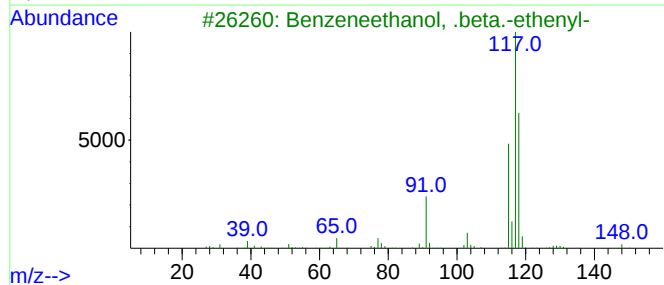
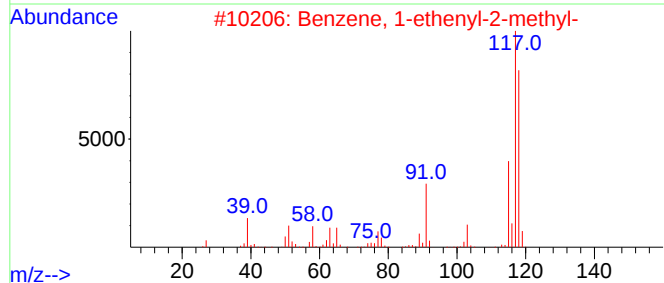
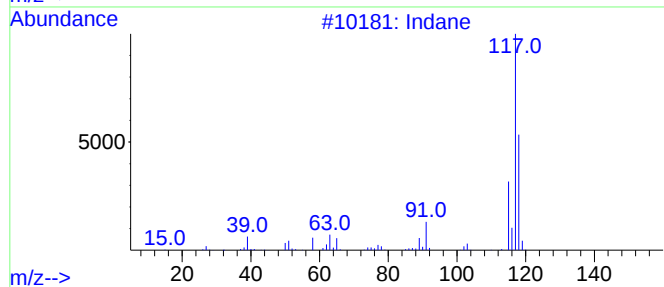
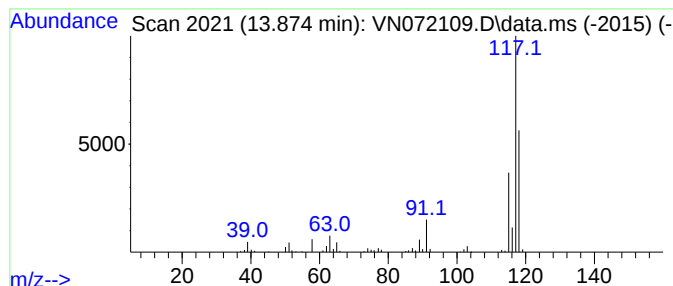
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.61 ug/l	340631	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
3			Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	78
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.134	21.8	ug/l	869187	1	8.080	1991320	50.0
Cyclobutane, me...	5.187	10.4	ug/l	415746	1	8.080	1991320	50.0
Cyclopentane, m...	7.145	9.9	ug/l	394803	1	8.080	1991320	50.0
Indane	13.874	6.6	ug/l	340631	4	13.668	2575670	50.0